

Tris(2-chloroethyl) phosphate  
115-96-8 | DTXSID5021411

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $2.07 \times 10^{-11}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $4.30 \times 10^{-1}$

**Confidence level:**  $8.17 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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Triethyl phosphate

**Measured:**  $5.53 \times 10^{-11}$

**Predicted:**  $4.26 \times 10^{-11}$

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Phosphoramidic acid, dimethyl-, dimethyl ester

**Measured:**  $3.19 \times 10^{-11}$

**Predicted:**  $2.75 \times 10^{-11}$

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Ethyl ethylcarbamate

**Measured:**  $1.44 \times 10^{-11}$

**Predicted:**  $1.58 \times 10^{-11}$

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N-Methylcarbamic acid, ethyl ester

**Measured:**  $8.30 \times 10^{-12}$

**Predicted:**  $1.01 \times 10^{-11}$

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Carbamic acid, ethyl-, methyl ester

**Measured:**  $1.05 \times 10^{-11}$

**Predicted:**  $1.06 \times 10^{-11}$